

Discretisation parameter and operator ordering in loop quantum cosmology with the cosmological constant

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In loop quantum cosmology, the Hamiltonian reduces to a finite difference operator. We study the initial singularity and the large volume limit against the ambiguities in the discretisation and the operator ordering within a homogeneous, isotropic and spatially flat model with the cosmological constant. We find that the absence of the singularity strongly depends on the choice of the operator ordering and the requirement for the absence singles out a very small class of orderings. Moreover we find a general ordering rule required for the absence of the singularity. We also find that the large volume limit naturally recovers a smooth wave function in the discretisation where each step corresponds to a fixed volume increment but not in the one where each step corresponds to a fixed area increment. If loop quantum cosmology is to be a phenomenological realisation of full loop quantum gravity, these results are important to fix the theoretical ambiguities.

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I. INTRODUCTION

Loop quantum gravity (LQG) is a background-independent nonperturbative quantum gravity. There, one quantises the Hamiltonian formulation of general relativity based on the $SU(2)$ connection A_a^i and the densitised triad E_i^a on the three-dimensional space, where a, b, \dots and i, j, \dots both run over 1, 2 and 3. a, b, \dots are tangent indices, while i, j, \dots are indices associated with a basis $\{\tau_i\}$ for the Lie algebra of $SU(2)$ Lie group and raised and lowered with Kronecker's delta δ_{ij} . The three-dimensional inverse metric is given by $q^{ab} = |\det E_k^c|^{-1} E_i^a E_j^b \delta^{ij}$. To quantise the system, LQG invokes holonomies $h_e = e^{\int_e A_a^i \tau_i dx^a}$ along an edge e and fluxes $\mathcal{E}_S = \int_S d^2\sigma n_a E_i^a \tau^i$ over a two-surface \mathcal{S} , where $d^2\sigma$ is the area element on \mathcal{S} and n_a is a unit normal to \mathcal{S} . There appears a nondimensional constant parameter γ , which is called the Barbero-Immirzi parameter and cannot be determined within the theory. The kinematical Hilbert space is spanned by the spin network states. The Hamiltonian as well as the area and the volume are constructed from holonomies and fluxes and act as operators on the kinematical Hilbert space. The Hilbert space is spanned by equivalence classes of the spin networks under diffeomorphisms or the s-knot states. See [1–3] for the basics and recent developments in LQG.

Loop quantum cosmology (LQC) [4] is a quantised minisuperspace model motivated by LQG. In traditional quantum cosmology [5], symmetry reduced models are quantised in the usual Schrödinger representation and the quantised Hamiltonian constraint yields the Wheeler-DeWitt (WDW) differential equation, while in LQC one uses the so-called polymer particle representation [6] which is unitary inequivalent to the Schrödinger representation and obtains a second order *difference equation* rather than the differential equation. Remarkably, Bojowald [7] demonstrated that there can be no big bang singularity in the following two aspects. First, the spectrum of the inverse scale factor operator is bounded from above. Second, the wave function of the universe can be uniquely extended beyond the point which was the initial singularity in classical theory. The above features have been first shown for a homogeneous, isotropic and spatially flat model and subsequently generalised to nonflat or anisotropic cases [4], although it is yet uncertain whether this can be generalised to inhomogeneous models (see e.g. [8, 9]).

In this paper, we visit the absence of the singularity in the presence of the cosmological constant against the quantisation ambiguities. In particular, we focus on the choice of the discretisation parameter λ which corresponds to

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the coordinate length of edges for the basic holonomies and the operator ordering in the Hamiltonian constraint. To study these issues, we fix the cosmological model to be homogeneous, isotropic and spatially flat with the cosmological constant. We first adopt the constant λ as in [7], for which the universe gains a fixed area quantum at each step and find that the absence of the singularity strongly depends on the operator ordering in the Hamiltonian. However, for this discretisation, we encounter a serious problem in the physical interpretation of the obtained wave function in the large volume limit. The problem is that the behaviour of the wave function obtained from the difference equation in LQC does not agree with that obtained from the WDW equation in the large volume limit. Since the effects of discreteness are dominant in the Planck scale physics but should disappear when the universe becomes large, the discrete wave function in LQC in the large volume is expected to have a correspondence to the smooth wave function which is a solution to the WDW equation. We see that this problem is resolved if λ is chosen to vary [10] so that the universe gains a fixed volume quantum and find that the absence of the singularity strongly depends on the operator ordering in the Hamiltonian also in this discretisation. It is already studied in detail how the large volume limit depends on the choice of the discretisation in the presence of matter fields by Nelson and Sakellariadou [11, 12] and the present result with the cosmological constant but without matter fields is consistent with theirs.

This paper is organised as follows. In Section II, we introduce the discretised Hamiltonian for a homogeneous, isotropic and spatially flat model with the cosmological constant. In Section III, we choose λ to be constant and derive the difference equation. Then, we demonstrate how the absence of the singularity depends on the choice of the operator ordering and numerically and analytically show the large volume limit is problematic. In Section IV, we vary λ appropriately and derive the difference equation. Then, we show that the large volume limit problem is resolved in this discretisation and also find that the absence of the singularity strongly depends on the choice of the operator ordering. Section V is devoted to discussion for the influence of the matter fields. In Section VI we conclude the paper. In this paper we use the units in which $c = \hbar = 1$.

II. LOOP QUANTUM COSMOLOGY

A. Hamiltonian constraint

In the present paper, we focus on a homogeneous, isotropic and spatially flat universe. In classical theory, the line element for such a spacetime is given by the flat Friedmann-Robertson-Walker (FRW) metric

$$ds^2 = -dt^2 + a(t)^2 (dx^2 + dy^2 + dz^2), \quad (2.1)$$

where $a(t)$ is called the scale factor. To remove the divergence coming from the volume integral we introduce an elementary cell \mathcal{V} on the three dimensional space. In this case, the gravitational Hamiltonian constraint is written as [13]

$$C_{\text{grav}} = \frac{1}{16\pi G\gamma^2} \int_{\mathcal{V}} d^3x \left(-\frac{1}{\sqrt{|\det E_i^a|}} \epsilon_{ijk} F_{ab}^i E^{aj} E^{bk} + 2\gamma^2 \sqrt{|\det E_i^a|} \Lambda \right), \quad (2.2)$$

where G , Λ , ϵ_{ijk} and $F_{ab}^i = \partial_a A_b^i - \partial_b A_a^i + \epsilon_{jk}^i A_a^j A_b^k$ are the gravitational constant, the cosmological constant, the Levi-Civita symbol and the curvature associated with the connection A_a^i , respectively. Although the cosmological constant might be an emergent object from some unknown effects, we incorporate it into the Hamiltonian as usual for simplicity. In the elementary cell \mathcal{V} , we define a time-independent fiducial flat metric \bar{q}_{ab} , an associated orthonormal triad $\{\bar{e}_i^a\}$ and cotriad $\{\bar{\omega}_a^i\}$. In the flat FRW universe, the connection A_a^i and the densitised triad E_i^a are given by

$$A_a^i = cV_0^{-(1/3)}\bar{\omega}_a^i, \quad E_i^a = pV_0^{-(2/3)}\sqrt{\bar{q}}\bar{e}_i^a, \quad (2.3)$$

where \bar{q} is the determinant of \bar{q}_{ab} , $c = V_0^{1/3} \text{sgn}(p)\gamma da/dt$, $|p| = V_0^{2/3}a^2$ and $V_0 = \int_{\mathcal{V}} d^3x \sqrt{\bar{q}}$. V_0 is thus the volume of the elementary cell with respect to the fiducial metric. In other words, $|p|$ is proportional to the physical area of the elementary cell and c is the conjugate momentum of p . The Poisson bracket between c and p takes the form $\{c, p\} = 8\pi G\gamma/3$. Now, the holonomy $h_i^{(\lambda)}$ along an edge parallel to \bar{e}_i^a is given by

$$h_i^{(\lambda)} = e^{\lambda c \tau_i}, \quad (2.4)$$

where λ is the coordinate length of the edge and $\{\tau_i\}$ are a basis for the Lie algebra of $\text{SU}(2)$ Lie group. The flux \mathcal{E}_S is simply given by $\mathcal{E}_S = pV_0^{-2/3}A_S$, where A_S is the area of the surface S [15]. Note that in defining the Hamiltonian

constraint operator, one traces over $SU(2)$ valued holonomies, and then there appears an ambiguity in choosing the irreducible representation to perform the trace. Here, we choose the spin $J = 1/2$ representation for simplicity. Then the holonomy becomes

$$h_i^{(\lambda)} = \cos(\lambda c/2) \mathbb{I} + 2 \sin(\lambda c/2) \tau_i, \quad (2.5)$$

where \mathbb{I} is the unit 2×2 matrix and $\{\tau_i\}$ are related to the Pauli matrices $\{\sigma_i\}$ via $2i\tau_i = \sigma_i$.

We rewrite the Hamiltonian constraint in terms of the flux p and the holonomy $h_k^{(\lambda)}$ as in the full theory. For the triad part of the first term in the constraint (2.2), we obtain

$$\epsilon_{ijk} \tau^i \frac{E^{aj} E^{bk}}{\sqrt{|\det E_i^a|}} = -\frac{2 \text{sgn}(p)}{8\pi G \gamma \lambda V_0^{\frac{2}{3}}} \bar{\epsilon}^{abc} \bar{\omega}_c^i \left(h_i^{(\lambda)} \left\{ \left(h_i^{(\lambda)} \right)^{-1}, V \right\} \right), \quad (2.6)$$

where $\bar{\epsilon}^{abc}$ is the Levi-Civita symbol, V is the volume and $\{\bullet, \bullet\}$ denotes the Poisson bracket. For the curvature F_{ab}^i , we rely on a standard prescription in gauge theories. We consider a loop α , which is a square \square_{ij} spanned by two triad vectors \bar{e}_i^a and \bar{e}_j^b of which each side is as long as λ in the coordinate length. Then, the ab component of the curvature is given by

$$\tau_i F_{ab}^i = \lim_{\text{Area} \rightarrow 0} \left(\frac{h_{\alpha}^{(\lambda)}{}_{ij} - \delta_{ij}}{\lambda^2 V_0^{\frac{2}{3}}} \right) \bar{\omega}_a^i \bar{\omega}_b^j, \quad (2.7)$$

where the holonomy $h_{\alpha}^{(\lambda)}{}_{ij}$ along $\alpha = \square_{ij}$ is the product of holonomies along the four edges,

$$h_{\alpha}^{(\lambda)}{}_{ij} = h_i^{(\lambda)} h_j^{(\lambda)} \left(h_i^{(\lambda)} \right)^{-1} \left(h_j^{(\lambda)} \right)^{-1}. \quad (2.8)$$

Substituting Eqs. (2.6), (2.7), and (2.8) into Eq. (2.2), C_{grav} can be expressed as

$$C_{\text{grav}} = \frac{1}{16\pi G \gamma^2} \left(-\frac{4 \text{sgn}(p)}{8\pi \lambda^3 G \gamma} \sum_{ijk} \epsilon^{ijk} \text{Tr} \left[h_i^{(\lambda)} h_j^{(\lambda)} \left(h_i^{(\lambda)} \right)^{-1} \left(h_j^{(\lambda)} \right)^{-1} h_k^{(\lambda)} \left\{ \left(h_k^{(\lambda)} \right)^{-1}, V \right\} \right] + 2\gamma^2 \Lambda V \right), \quad (2.9)$$

where we have used the relation

$$\tau_i \tau_j = \frac{1}{2} \epsilon_{ijk} \tau^k - \frac{1}{4} \delta_{ij} \mathbb{I}. \quad (2.10)$$

To quantise the Hamiltonian, we replace $h_i^{(\lambda)}$ and p with the corresponding operators. The kinematical Hilbert space is defined by $\mathcal{H}_{\text{kin}}^{\text{grav}} = L^2(\mathbb{R}_{\text{Bohr}}, d\mu_{\text{Bohr}})$, where \mathbb{R}_{Bohr} is the Bohr compactification of the real line and $d\mu_{\text{Bohr}}$ is the Haar measure on it [1, 2, 6, 10]. An orthonormal basis for the kinematical Hilbert space is given by a set of eigenstates $\{|\mu\rangle\}$ of \hat{p} , which satisfy the orthonormality relations $\langle \mu_1 | \mu_2 \rangle = \delta_{\mu_1 \mu_2}$. The action of the triad operator \hat{p} on the state $|\mu\rangle$ is given by

$$\hat{p}|\mu\rangle = \frac{8\pi\gamma l_{\text{Pl}}^2}{6} \mu |\mu\rangle, \quad (2.11)$$

where $l_{\text{Pl}} := \sqrt{G}$ is the Planck length. That is, the eigenvalues of \hat{p} are labelled by the dimensionless parameter μ . The states $\{|\mu\rangle\}$ are also eigenstates of the volume operator $\hat{V} = \widehat{|p|^{3/2}}$:

$$\hat{V}|\mu\rangle = \widehat{|p|^{3/2}}|\mu\rangle = V_{\mu}|\mu\rangle, \quad (2.12)$$

where

$$V_{\mu} = \left(\frac{8\pi\gamma l_{\text{Pl}}^2}{6} |\mu| \right)^{3/2}. \quad (2.13)$$

Using Eqs. (2.4) and (2.9) and replacing the Poisson bracket with a commutator, after some calculation, we find

$$\hat{C}_{\text{grav}} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i (\text{sgn}(p))}{8\pi \gamma l_{\text{Pl}}^2} \frac{1}{\lambda^3} \widehat{\sin^2 \frac{\lambda c}{2} \cos^2 \frac{\lambda c}{2}} \left[\sin \frac{\lambda c}{2} V \cos \frac{\lambda c}{2} - \cos \frac{\lambda c}{2} V \sin \frac{\lambda c}{2} \right] + 2\gamma^2 \Lambda \hat{V} \right), \quad (2.14)$$

where the operator ordering is fixed for simplicity. The ambiguity in the ordering will be discussed later. Note that λ itself is an operator in general. It should be noted that in LQC we do not take the limit $\lambda \rightarrow 0$. Later we will discuss the physical motivation for this setting.

B. Discretisation ambiguity

In full LQG, the geometry is quantised through the area and volume operators. To define the area operator $\widehat{\mathbf{A}}(\mathcal{S})$ for a two-surface \mathcal{S} , we partition \mathcal{S} into N small two-surfaces $\{\mathcal{S}_n\}$ such that $\cup_n \mathcal{S}_n = \mathcal{S}$. For sufficiently large N , there is $\{\mathcal{S}_n\}$ such that no \mathcal{S}_n will contain more than one intersection with the graph Γ of the spin network $|\mathcal{S}\rangle$. The sum over n reduces to a sum over the intersection points between \mathcal{S} and Γ and is independent of N for sufficiently large N . Then, the action of the area operator becomes

$$\widehat{\mathbf{A}}(\mathcal{S})|\mathcal{S}\rangle = 4\pi\gamma l_{\text{Pl}}^2 \sum_i \sqrt{2j_i^u(j_i^u + 1) + 2j_i^d(j_i^d + 1) - j_i^t(j_i^t + 1)}|\mathcal{S}\rangle, \quad (2.15)$$

where $\{i\}$ label the intersection points between the graph Γ and the two-surface \mathcal{S} , the indices u , d and t stand for the edges upward, downward and tangential to the \mathcal{S} , respectively, and the positive half integers j_i^u , j_i^d and j_i^t are the spins of the links labelled by i [16]. Thus, there appears the smallest area $\Delta = 2\sqrt{3}\pi\gamma l_{\text{Pl}}^2$. For the volume operator \widehat{V} for a three-volume \mathcal{R} , we take a similar strategy. We partition the three-volume \mathcal{R} into cubes $\{\mathcal{R}_n\}$ of the coordinate volume ϵ^3 and for sufficiently small ϵ no cube will contain more than one node. The volume operator has a nontrivial action only on nodes and hence it will no longer depend on the value of ϵ . Then, it turns out that the spin network state is an eigenstate of the volume operator and the eigenvalue is given by the sum over the nodes which are contained in the three-volume \mathcal{R} and at least quadrivalent. Similarly, we define the quantised Hamiltonian, which has a nontrivial action only on nodes. Thus, for sufficiently small ϵ , the action of the quantised Hamiltonian will not depend on ϵ .

In LQC, however, we leave the parameter λ of the discretisation nonzero finite. In fact, we are forced to do so in the present formulation of LQC because there is no operator corresponding to c . On the other hand, the physical results seem to depend on the choice of λ . From this point of view, there is no first principle within the formulation of LQC about how to choose the nonzero finite value for the discretisation parameter λ . We should probably fix the discretisation parameter λ (and other quantisation ambiguities) in LQC so that LQC can reproduce the features that full LQG should have.

To see how λ is kept nonzero, we see the following relation:

$$\widehat{|p|}h_i^{(\lambda)} = \frac{8\pi}{6}\gamma l_{\text{Pl}}^2|\lambda|h_i^{(\lambda)}. \quad (2.16)$$

Note that $|p|$ is the physical area of the elementary cell. Since the curvature in the Hamiltonian invokes the holonomy $h_{\alpha}^{(\lambda)}{}_{ij}$ along the square \square_{ij} , it would be reasonable to assume that each edge of this square is quantised so that the holonomy along each edge intersects the smallest area Δ of full LQG. This argument motivates us to choose λ to be a constant μ_0 of order unity. This choice is adopted in Refs. [7, 15, 17]. The value for μ_0 to fulfill this requirement exactly is $3\sqrt{3}/2$. The basic operator which appears in the Hamiltonian is $\exp(\widehat{i\mu_0 c}/2)$ and this acts on $|\mu\rangle$ as follows:

$$\widehat{e^{i\mu_0 c/2}}|\mu\rangle = |\mu + \mu_0\rangle. \quad (2.17)$$

This means that the eigenvalues of $\widehat{\mu}$ for the states which appear in the Hamiltonian constraint are spaced at constant intervals. Note that as seen in Eq. (2.17), the operator $\exp(\widehat{i\mu_0 c}/2)$ drags the state $|\mu\rangle$ by the parameter length μ_0 along the vector $d/d\mu$. Then, we can rewrite Eq. (2.17) as

$$\widehat{e^{i\mu_0 c/2}}|\mu\rangle = e^{\mu_0(d/d\mu)}|\mu\rangle. \quad (2.18)$$

We call this choice of the parameter λ the equi-area discretisation.

However, this is not the only possible choice. Since the curvature in the Hamiltonian invokes the holonomy $h_{\alpha}^{(\lambda)}{}_{ij}$ along the square \square_{ij} , it would also be reasonable to assume that the area of this square is set to be the smallest area Δ of full LQG. This motivates us to choose λ to be a function $\lambda = \bar{\mu}(p)$ such that

$$\bar{\mu}^2|p| = \Delta. \quad (2.19)$$

This gives another choice of the parameter λ . In this case, from Eq. (2.11) we find that $\bar{\mu}$ depends on μ as follows:

$$\bar{\mu}^2|\mu| = \frac{3\sqrt{3}}{2}. \quad (2.20)$$

Similarly to Eq. (2.18), we can rewrite the operator $\exp(i\bar{\mu}c/2)$ as

$$\widehat{e^{i\bar{\mu}c/2}}|\mu\rangle = e^{\bar{\mu}(d/d\mu)}|\mu\rangle. \quad (2.21)$$

If we introduce a variable v satisfying

$$dv = \frac{1}{\bar{\mu}}d\mu, \quad (2.22)$$

we can rewrite the right hand side of Eq. (2.21) as

$$e^{\bar{\mu}\frac{d}{d\mu}}|\mu\rangle = e^{\frac{d}{dv}}|\mu\rangle. \quad (2.23)$$

This means that if we adopt the v -representation of the wave function, the action of the Hamiltonian becomes simple. The explicit integration of Eq. (2.22) using Eq. (2.20) yields

$$v = \text{sgn}(\mu)K|\mu|^{\frac{3}{2}}, \quad (2.24)$$

where $K = 2\sqrt{2}/(3\sqrt{3\sqrt{3}})$. We should note that v is proportional to the volume V . This choice is adopted in Ref. [10]. In this case, it is more convenient to use the eigenstates $|v\rangle$ of the volume operator \hat{V} to see the action of the Hamiltonian constraint. The eigenstate $|v\rangle$ satisfies

$$\hat{V}|v\rangle = V_v|v\rangle, \quad (2.25)$$

where

$$V_v = \left(\frac{8\pi}{6}\gamma l_{\text{Pl}}^2\right)^{3/2} \frac{|v|}{K}. \quad (2.26)$$

The basic operator which appears in the Hamiltonian is $\widehat{e^{i\bar{\mu}c/2}}$ and its action on $|v\rangle$ is given by

$$\widehat{e^{i\bar{\mu}c/2}}|v\rangle = |v+1\rangle. \quad (2.27)$$

Consequently, the Hamiltonian constraint involves the volume eigenstates of which the eigenvalues are equally spaced. In other words, the spectrum of the volume operator is distributed at equidistant intervals in volume. Thus, we will call this discretisation the equi-volume discretisation. Note that since $\lambda = \bar{\mu}(p)$ depends on p , λ should be treated as an operator in quantum theory.

III. EQUI-AREA DISCRETISATION

A. Absence of singularity and operator ordering

First we concentrate on the equi-area discretisation. The holonomy operator acts on $|\mu\rangle$ as

$$\widehat{h_k^{(\mu_0)}}|\mu\rangle = \frac{1}{2}(|\mu + \mu_0\rangle + |\mu - \mu_0\rangle)\mathbb{I} + \frac{1}{i}(|\mu + \mu_0\rangle - |\mu - \mu_0\rangle)\tau_k. \quad (3.1)$$

Even within this discretisation, there are many possible choices of the operator ordering. To make the notation simple, we put

$$\widehat{F} = \sin^2\frac{\mu_0 c}{2}\cos^2\frac{\mu_0 c}{2}, \quad \widehat{EE} = \sin\frac{\mu_0 c}{2}V\cos\frac{\mu_0 c}{2} - \cos\frac{\mu_0 c}{2}V\sin\frac{\mu_0 c}{2}, \quad (3.2)$$

where F and EE relate to the squared holonomy $h_{\alpha ij}$ (2.8) and the Poisson bracket $h_i\{(h_i)^{-1}, V\}$ in Eq. (2.6), respectively. For simplicity, hereafter we fix the ordering for the contents of \widehat{F} and \widehat{EE} , and then there are two choices of the operator ordering in the Hamiltonian constraint operator as $\widehat{F}\widehat{EE}$ or $\widehat{EE}\widehat{F}$. We first consider the operator ordering adopted in Ref. [7]:

$$\widehat{C}_{\text{grav}} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i(\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2 \mu_0^3} \widehat{F}\widehat{EE} + 2\gamma^2 \Lambda \widehat{V} \right). \quad (3.3)$$

Then the action of the operator on a state $|\Psi\rangle$ leads to the difference equation, i.e., $\langle\mu|\widehat{C}_{\text{grav}}|\Psi\rangle = 0$ yields

$$|V_{\mu+5\mu_0} - V_{\mu+3\mu_0}| \Psi(\mu + 4\mu_0) - \left(2|V_{\mu+\mu_0} - V_{\mu-\mu_0}| - \frac{16\pi\gamma^3 l_{\text{Pl}}^2 \mu_0^3}{3} \Lambda V_\mu \right) \Psi(\mu) + |V_{\mu-3\mu_0} - V_{\mu-5\mu_0}| \Psi(\mu - 4\mu_0) = 0, \quad (3.4)$$

where $\Psi(\mu) = \langle\mu|\Psi\rangle$. If we interpret the triad coefficient p as an internal time, we can regard the difference equation (3.4) as an evolution equation with respect to the discrete time. We can see that $\Psi(0)$ disappears for $\mu = 0$ and $\pm 4\mu_0$. For this reason, the solution can be uniquely extended beyond the classical singularity $\mu = 0$. That is, given some two initial data $\Psi(\epsilon + 4N\mu_0)$ and $\Psi(\epsilon + 4(N+1)\mu_0)$ for $\epsilon \in (0, 4\mu_0)$ and a natural number N , one can uniquely determine the values $\Psi(\epsilon + 4n\mu_0)$ for $n = 0, \pm 1, \pm 2, \dots$. For the $\epsilon = 0$ case, given some two initial data $\Psi(4N\mu_0)$ and $\Psi(4(N+1)\mu_0)$, the difference equation (3.4) generates $\Psi(4n\mu_0)$ for $n = 1, 2, \dots$ but the set of $\Psi(8\mu_0)$ and $\Psi(4\mu_0)$ does not generally satisfy Eq. (3.4). This means that $\Psi(4N\mu_0)$ and $\Psi(4(N+1)\mu_0)$ are constrained, and once this is satisfied, we can uniquely determine the values $\Psi(4n\mu_0)$ for $n = \pm 1, \pm 2, \dots$. Thus, we can conclude that the system has no initial singularity in this operator ordering. Although $\Psi(0)$ is left undetermined in Eq. (3.4), we can determine unambiguously the discrete evolution beyond $\mu = 0$. That is, the unique quantum evolution is not affected in spite of the undetermined value at $\mu = 0$, which was the initial singularity in classical theory. This ambiguity is fixed so that $\Psi(0) = 0$ in Ref. [7] and we also use this value in our numerical analysis.

Here we should note the superselection of the kinematical Hilbert space. As seen from Eq. (3.4), a subspace \mathcal{H}_ϵ with a fixed parameter $\epsilon \in [0, 4\mu_0)$ spanned by a basis $\{|\mu\rangle : \mu = \epsilon + 4n\mu_0, n \in \mathbb{Z}\}$ of the kinematical Hilbert space $\mathcal{H}_{\text{kin}}^{\text{grav}}$ are closed with respect to the action of the Hamiltonian constraint. More precisely, the kinematical Hilbert space is naturally decomposed into the sectors with respect to the action of the Hamiltonian constraint as

$$\mathcal{H}_{\text{kin}}^{\text{grav}} = \bigoplus_{\epsilon \in [0, 4\mu_0)} \mathcal{H}_\epsilon.$$

We refer to this decomposition as the superselection and to these subspaces as the superselection sectors. The superselection in LQC indicates that for each sector we can fix the value of ϵ and work within this sector \mathcal{H}_ϵ . Since there is no initial singularity for the sectors with $\epsilon \neq 0$ in this case, we only have to choose the sector with $\epsilon = 0$ to study the presence or absence of the initial singularity at $\mu = 0$. On the other hand, when we consider the large μ limit, the value of ϵ does not affect the qualitative behaviour of $\Psi(\mu)$ and hence we can focus on the sector with $\epsilon = 0$ again. This is also the case in the equi-volume discretisation.

Next we consider the following operator ordering:

$$\widehat{C}_{\text{grav}} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i (\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2 \mu_0^3} \widehat{EE}\widehat{F} + 2\gamma^2 \Lambda \widehat{V} \right). \quad (3.5)$$

Then, the difference equation is given by

$$|-V_{\mu+\mu_0} + V_{\mu-\mu_0}| (\Psi(\mu + 4\mu_0) - 2\Psi(\mu) + \Psi(\mu - 4\mu_0)) + \frac{16\pi\gamma^3 l_{\text{Pl}}^2 \mu_0^3}{3} \Lambda V_\mu \Psi(\mu) = 0. \quad (3.6)$$

We can see that Eq. (3.6) becomes trivial for $\mu = 0$ and hence we cannot determine $\Psi(-4\mu_0)$ from $\Psi(4\mu_0)$ and $\Psi(0)$. This fact indicates that we cannot determine all $\Psi(\mu)$ through $\mu = 0$ from the data $\Psi(\mu)$ for $\mu > 0$. In this sense, the model contains the initial singularity at $\mu = 0$, beyond which the evolution cannot be uniquely extended. This means that the absence of the singularity depends on the choice of the operator ordering in the quantisation of the Hamiltonian.

B. Large volume limit problem

In this section, we shall see the large- μ behaviour of the wave function $\Psi(\mu)$ determined by the difference equation and discuss its physical implication. Since the effects of the discreteness are dominant in the Planck scale physics but should disappear when the universe becomes large, in LQC the discrete wave function in the large volume is expected to be well approximated by a smooth wave function. If this naive expectation is valid, it is natural to think that the smooth wave function is described by a solution to the WDW equation which is obtained by quantising the system in the usual Schrödinger representation. We give a brief derivation of the WDW equation in Appendix A.

To see the large- μ behaviour of the discretised wave function $\Psi(\mu)$, we numerically solve the difference equation (3.4). We first choose the initial values $\Psi(-4\mu_0)$ and $\Psi(0)$, and then determine $\Psi(4n\mu_0)$ for $n = 1, 2, \dots$ by the

difference equation. Here we define the dimensionless cosmological constant as $\tilde{\Lambda} = (16\pi/3)\gamma^3 l_{\text{Pl}}^2 \Lambda$. In the numerical calculation below, we set $\tilde{\Lambda}\mu_0^3 = 0.005$ and these initial values as $\Psi(-4\mu_0) = -1$ and $\Psi(0) = 0$, where the values have no particular meaning and are selected to make the plots of the wave function visible. Figs. 1(a) and 1(b) show the wave function $\Psi(\mu)$ as a function of $\mu = 4n\mu_0$, and Fig. 1(c) is for the logarithmic scale of $|\Psi(\mu)|$. As Fig. 1(a) illustrates, the wave function $\Psi(\mu)$ can be regarded as the sampling of a decaying sinusoidal oscillation at the points sufficiently near the origin. However, as seen from Fig. 1(b), $\Psi(\mu)$ drastically changes its behaviour at $\mu \simeq 2400\mu_0$, so that $\Psi(\mu)$ flips its sign at each step and its absolute value grows up very rapidly for $\mu \gtrsim 2400\mu_0$. We can see from Fig. 1(c) that $|\Psi(\mu)|$ grows approximately exponentially for $\mu \gtrsim 2400\mu_0$.

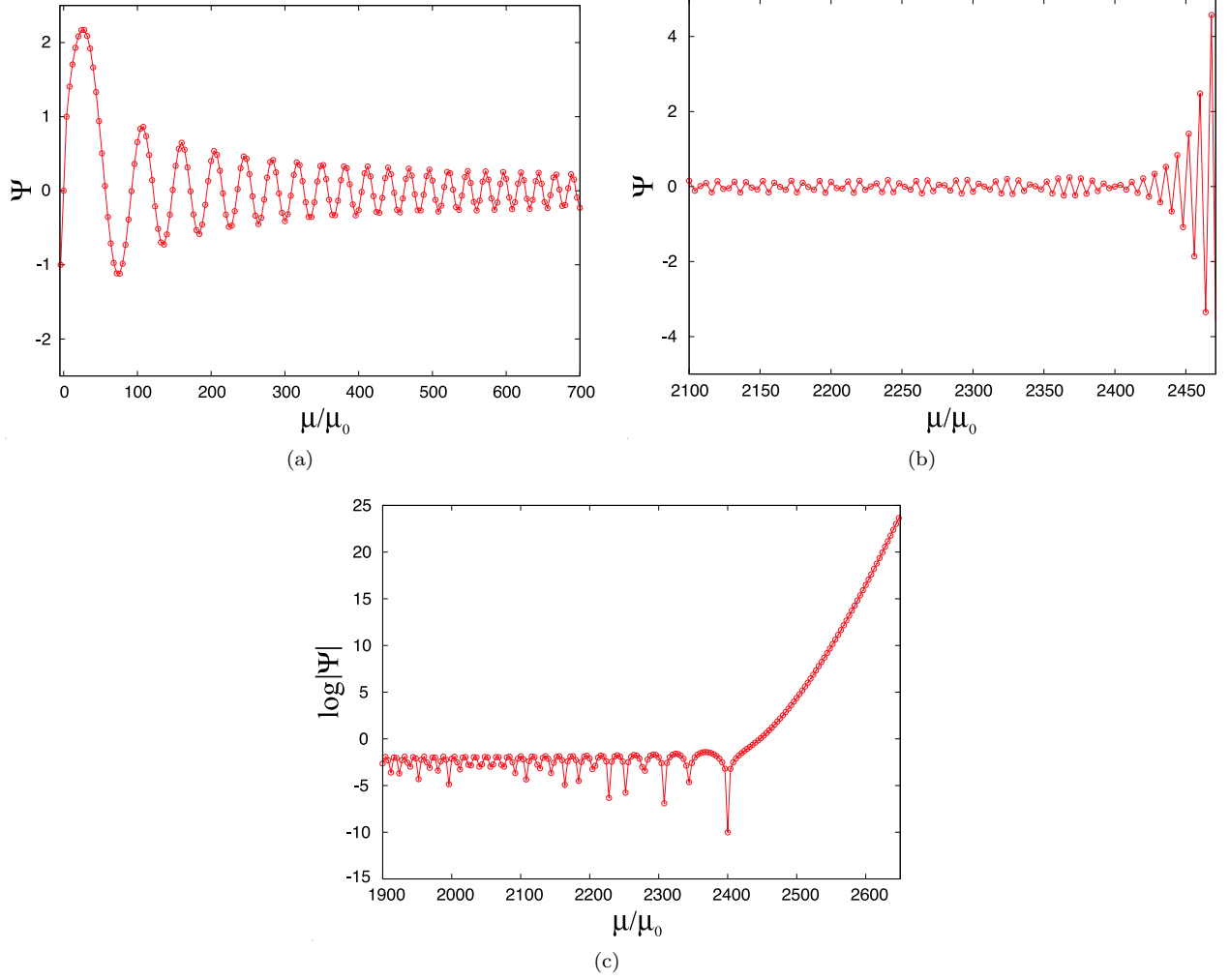


FIG. 1: The wave function $\Psi(\mu)$ for (a) $0 \leq \mu/\mu_0 \leq 700$ and (b) $2100 \leq \mu/\mu_0 \lesssim 2450$, and (c) the logarithmic scale of its absolute value are plotted as a function of μ with $\tilde{\Lambda}\mu_0^3 = 0.005$, where we choose the initial values as $\Psi(-4\mu_0) = -1$ and $\Psi(0) = 0$.

This behaviour can be deduced from the following simple argument. We have the recursive relation (3.4). For $\mu \gg \mu_0$, we have

$$\Psi(\mu + 4\mu_0) - \left(2 - \frac{1}{3}\mu\mu_0^2\tilde{\Lambda}\right)\Psi(\mu) + \Psi(\mu - 4\mu_0) = 0. \quad (3.7)$$

If $|\mu\mu_0^2\tilde{\Lambda}/6| \ll 1$, it is easily found that the solution is given by

$$\Psi(\mu_0 + 4n\mu_0) \approx An + B, \quad (3.8)$$

where A and B are constants. However, if $|\mu\mu_0^2\tilde{\Lambda}/6| \gg 1$, in the present setting, we generally get a solution for which the last term on the left hand side of Eq. (3.7) can be neglected, i.e.,

$$\Psi(\mu + 4\mu_0) \approx \left(2 - \frac{1}{3}\mu\mu_0^2\tilde{\Lambda}\right) \Psi(\mu). \quad (3.9)$$

For $|\mu\mu_0^2\tilde{\Lambda}/6| \gg 1$, the factor $(2 - \mu\mu_0^2\tilde{\Lambda}/3)$ is negative and positive if the cosmological constant is positive and negative, respectively. In both cases, its absolute value is much larger than unity from the assumption. Thus, $\Psi(\mu)$ increases its absolute value at each step by the factor which is much larger than unity and the growth is approximately exponential. It is clear that the latter case cannot be regarded as smooth in spite of the very large volume. We can expect that this peculiar behaviour becomes prominent for $\mu \simeq 9\mu_0^{-2}\tilde{\Lambda}^{-1}$ for $\tilde{\Lambda} > 0$ and this is consistent with the numerical result plotted in Fig. 1.

On the other hand, for $\mu \gg \mu_0$, the difference equation (3.4) can be approximated by the following WDW equation under the assumption that the wave function varies sufficiently slowly (see Appendix B for a detailed derivation):

$$\frac{d^2}{d\mu^2} (\sqrt{\mu}\Psi(\mu)) + \frac{\pi\gamma^3 l_{\text{Pl}}^2}{9} \mu^{3/2} \Lambda \Psi(\mu) = 0. \quad (3.10)$$

The general solution of the differential equation (3.10) for $\mu \geq 0$ takes the form

$$\Psi(\mu) = \mu^{-\frac{1}{2}} \left[C_1 \text{Ai} \left(-\alpha_1^{\frac{1}{3}} \mu \right) + C_2 \text{Bi} \left(-\alpha_1^{\frac{1}{3}} \mu \right) \right], \quad (3.11)$$

where C_1 and C_2 are arbitrary constants, Ai and Bi are the Airy functions and we have defined $\alpha_1 := (\pi/9)\gamma^3 l_{\text{Pl}}^2 \Lambda$. We present the WDW equations and its general solutions for some operator orderings in Appendix A. In the large $\alpha_1^{\frac{1}{3}} \mu$, the above function approaches a decaying sinusoidal curve. Thus, the behaviour of the solution, which is plotted in Fig. 1, to the difference equation (3.4) is quite different from that of the solution (3.11) to the differential equation (3.10) even when the volume of the universe becomes large. In other words, in the equi-area discretisation, the solution of the difference equation cannot be regarded as a smooth wave function for large μ in the presence of the cosmological constant. We refer to this problem as *the large-volume limit problem*.

IV. EQUI-VOLUME DISCRETISATION

A. Resolution of the large volume limit problem

In this section, we shall consider the large volume limit in the equi-volume discretisation. We should note that the Hamiltonian constraint is written as

$$C_{\text{grav}} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i(\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2} \widehat{\frac{1}{\bar{\mu}^3}} \sin^2 \frac{\bar{\mu}c}{2} \cos^2 \frac{\bar{\mu}c}{2} \left[\sin \left(\frac{\bar{\mu}c}{2} \right) V \cos \left(\frac{\bar{\mu}c}{2} \right) - \cos \left(\frac{\bar{\mu}c}{2} \right) V \sin \left(\frac{\bar{\mu}c}{2} \right) \right] + 2\gamma^2 \Lambda \widehat{V} \right), \quad (4.1)$$

where the ambiguity in the operator ordering is neglected. Since $\bar{\mu}$ is a function of p , $1/\bar{\mu}^3$ becomes also an operator in the quantisation. We put

$$\widehat{F} = \sin^2 \frac{\bar{\mu}c}{2} \cos^2 \frac{\bar{\mu}c}{2}, \quad \widehat{EE} = \sin \left(\frac{\bar{\mu}c}{2} \right) V \cos \left(\frac{\bar{\mu}c}{2} \right) - \cos \left(\frac{\bar{\mu}c}{2} \right) V \sin \left(\frac{\bar{\mu}c}{2} \right). \quad (4.2)$$

We first choose the following operator ordering:

$$C_{\text{grav}} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i(\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2} \widehat{F} \widehat{\frac{1}{\bar{\mu}^3}} \widehat{EE} + 2\gamma^2 \Lambda \widehat{V} \right), \quad (4.3)$$

and we will see the other choices in the next section.

As we have seen in Sec.IIB, in this case, it is convenient to use a new label v instead of μ . We rewrite $\widehat{1/\bar{\mu}^3}$ in terms of \widehat{V} as

$$\widehat{\frac{1}{\bar{\mu}^3}} = \left(\frac{6}{8\pi\gamma l_{\text{Pl}}^2} \right)^{3/2} \frac{K\widehat{V}}{\sqrt{3}}, \quad (4.4)$$

by using Eqs. (2.11), (2.19) and (2.24). Then, the Hamiltonian constraint yields the following difference equation:

$$|v+4| ||v+3| - |v+5|| \Phi(v+4) - \left(2|v| ||v-1| - |v+1|| - \frac{16\sqrt{3}\pi}{3} \gamma^3 l_{\text{Pl}}^2 \Lambda |v| \right) \Phi(v) + |v-4| ||v-5| - |v-3|| \Phi(v-4) = 0, \quad (4.5)$$

where $\Phi(v) = \langle v | \Phi \rangle$. We numerically obtain the solution of the above difference equation with $\sqrt{3}\tilde{\Lambda} = 0.1$ from the initial values $\Phi(-4) = -1$ and $\Phi(0) = 0$. Again, we have chosen these values to make the plots visible. The obtained wave function $\Phi(v)$ is plotted in Figs. 2(a) and 2(b). We see from these figures that the discretised wave function oscillates and can be regarded as the sampling of a smooth sinusoidal curve for large v . This means that the large volume limit problem in the equi-area discretisation is resolved in the equi-volume discretisation. Indeed, as presented in Appendix B, the difference equation (4.5) can be approximated by the WDW equation

$$\frac{d^2}{dv^2}(|v|\Phi(v)) + \frac{4\pi}{81K^2} \gamma^3 l_{\text{Pl}}^2 \Lambda |v| \Phi(v) = 0, \quad (4.6)$$

and the general solution is written as

$$\Phi(v) = \frac{1}{v} \left(C_1 e^{i\sqrt{\alpha_2}v} + C_2 e^{-i\sqrt{\alpha_2}v} \right), \quad (4.7)$$

where C_1 and C_2 are arbitrary constants and we have defined $\alpha_2 = \frac{4\pi}{81K^2} \gamma^3 l_{\text{Pl}}^2 \Lambda$. The wave function plotted in Fig. 2 has good agreement with the solution (4.7) for large v .

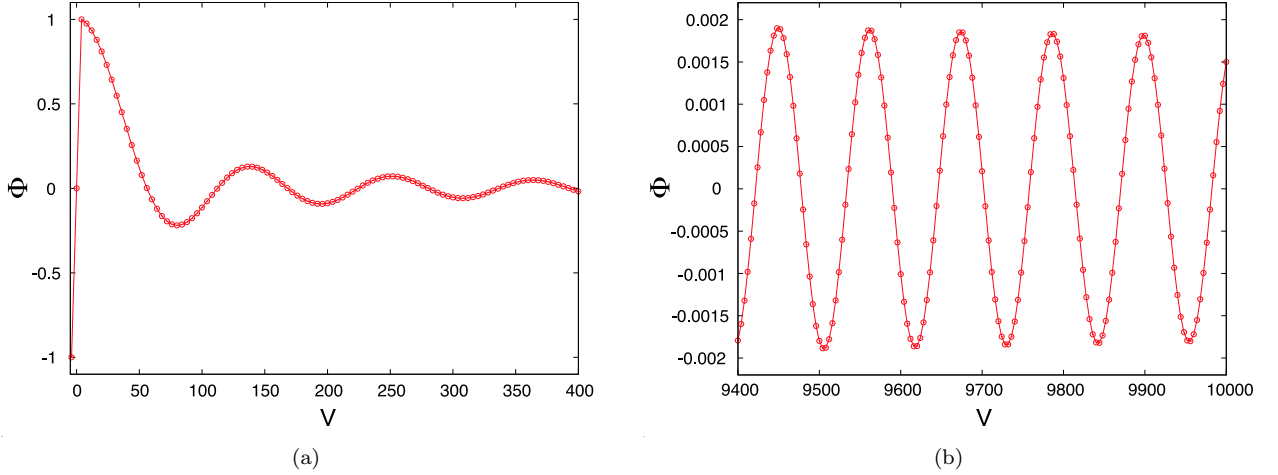


FIG. 2: The wave function $\Phi(v)$ for (a) $0 \leq v \leq 400$ and (b) $9400 \leq v \leq 10000$ are plotted as a function of $v = 4n$ with $\sqrt{3}\tilde{\Lambda} = 0.1$, where we choose the initial values as $\Phi(-4) = -1$ and $\Phi(0) = 0$.

We can also analytically show that the large volume limit should be resolved in this discretisation. For $v \gg 1$, we can approximate Eq. (4.5) by

$$\Phi(v+4) - 2(1 - C\tilde{\Lambda})\Phi(v) + \Phi(v-4) = 0, \quad (4.8)$$

where $C = 2/(27K^2)$. The characteristic equation for this recursive relation is the following:

$$x^2 - 2(1 - C\tilde{\Lambda})x + 1 = 0. \quad (4.9)$$

The roots are given by

$$x = (1 - C\tilde{\Lambda}) \pm \sqrt{(1 - C\tilde{\Lambda})^2 - 1}. \quad (4.10)$$

From the above, we can deduce the large- v behaviour of $\Phi(v)$. For $0 < C\tilde{\Lambda} < 2$, $\Phi(4n)$ purely oscillates sinusoidally. For $C\tilde{\Lambda} < 0$ or $C\tilde{\Lambda} > 2$, it is generally dominated by the exponential growth. For $C\tilde{\Lambda} = 0$, $\Phi(4n) = An + B$, where A and B are constants. For $C\tilde{\Lambda} = 2$, $\Phi(4n+4) + \Phi(4n) = (-1)^n D$, where D is a constant. Thus, if $|C\tilde{\Lambda}| \ll 1$, which is realistic in our Universe, $\Phi(4n)$ changes very slowly at each step whether it oscillates with the angular velocity $\sim \sqrt{C\tilde{\Lambda}}$ or grows exponentially with the growth rate $\sim \sqrt{C\tilde{\Lambda}}$. This means that we can physically regard $\Phi(v)$ as a smooth wave function in the large volume limit.

B. Absence of singularity and operator ordering

In this section, we shall discuss the initial singularity in the equi-volume discretisation. We here demonstrate the following four typical types of the operator ordering in the Hamiltonian constraint in the equi-volume discretisation and show that the existence or absence of the initial singularity depends on the choice of the operator ordering.

$$\widehat{C}_{\text{grav}}^{(a)} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i(\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2} \widehat{F} \frac{1}{\widehat{\mu}^3} \widehat{E}\widehat{E} + 2\gamma^2 \Lambda \widehat{V} \right), \quad (4.11a)$$

$$\widehat{C}_{\text{grav}}^{(b)} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i(\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2} \frac{1}{\widehat{\mu}^3} \widehat{F} \widehat{E}\widehat{E} + 2\gamma^2 \Lambda \widehat{V} \right), \quad (4.11b)$$

$$\widehat{C}_{\text{grav}}^{(c)} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i(\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2} \widehat{E}\widehat{E} \frac{1}{\widehat{\mu}^3} \widehat{F} + 2\gamma^2 \Lambda \widehat{V} \right), \quad (4.11c)$$

$$\widehat{C}_{\text{grav}}^{(d)} = \frac{1}{16\pi l_{\text{Pl}}^2 \gamma^2} \left(\frac{96i(\text{sgn}(p))}{8\pi\gamma l_{\text{Pl}}^2} \widehat{E}\widehat{E} \widehat{F} \frac{1}{\widehat{\mu}^3} + 2\gamma^2 \Lambda \widehat{V} \right). \quad (4.11d)$$

We call the above four types of the orderings (a), (b), (c) and (d). Note that $\widehat{E}\widehat{E}$ and $1/\widehat{\mu}^3$ are commutative with each other. We can also take different orderings. For example, $1/\widehat{\mu}^3$ could be divided into two and put on both sides of \widehat{F} . We will discuss these orderings later.

The above Hamiltonian constraints for orderings (a) - (d) yield respectively the following difference equations:

$$\begin{aligned} & |v+4| ||v+3| - |v+5| \Phi(v+4) \\ & - \left(2|v| ||v-1| - |v+1| - \frac{128\pi}{81} \gamma^3 \frac{l_{\text{Pl}}^2}{K^2} \Lambda |v| \right) \Phi(v) + |v-4| ||v-5| - |v-3| \Phi(v-4) = 0, \end{aligned} \quad (4.12a)$$

$$\begin{aligned} & |v| ||v+5| - |v+3| \Phi(v+4) \\ & - \left(2|v| ||v+1| - |v-1| - \frac{128\pi}{81} \gamma^3 \frac{l_{\text{Pl}}^2}{K^2} \Lambda |v| \right) \Phi(v) + |v| ||v-3| - |v-5| \Phi(v-4) = 0, \end{aligned} \quad (4.12b)$$

$$\begin{aligned} & |v| ||v+1| - |v-1| \Phi(v+4) \\ & - \left(2|v| ||v+1| - |v-1| - \frac{128\pi}{81} \gamma^3 \frac{l_{\text{Pl}}^2}{K^2} \Lambda |v| \right) \Phi(v) + |v| ||v+1| - |v-1| \Phi(v-4) = 0, \end{aligned} \quad (4.12c)$$

$$\begin{aligned} & |v+4| ||v+1| - |v-1| \Phi(v+4) \\ & - \left(2|v| ||v+1| - |v-1| - \frac{128\pi}{81} \gamma^3 \frac{l_{\text{Pl}}^2}{K^2} \Lambda |v| \right) \Phi(v) + |v-4| ||v+1| - |v-1| \Phi(v-4) = 0. \end{aligned} \quad (4.12d)$$

The WDW equations obtained by the approximation of the difference equations (4.12a)-(4.12d) are presented in Appendix B. We can see that $\Phi(0)$ disappears in any of these equations. However, only in Eq. (4.12a), $\Phi(4)$ can be directly related to $\Phi(-4)$. This leads to the following conclusion. Suppose that we are given $\Phi(v)$ for all $v > 0$. Then, only ordering (a) among the above four choices determines $\Phi(v)$ for all $v < 0$. For the other choices, the difference equation does not determine $\Phi(4n)$ for $n = -1, -2, -3, \dots$. In this sense, the absence of the singularity is possible in and only in ordering (a) among the choices (a)-(d). Thus, among the six models demonstrated in the present paper, the model with the equi-volume discretisation and ordering (a) is the only model where the initial singularity is absent and has the large volume limit as a smooth wave function. In ordering (a), if only we fix $\Phi(4)$, we can determine $\Phi(4n)$ for $n = \pm 1, \pm 2, \dots$. As in the equi-area discretisation, although $\Phi(0)$ is left undetermined, this does not affect the unique quantum evolution beyond $v = 0$.

Moreover, we can find a general ordering rule required for the absence of the singularity : If the volume operator \widehat{V} or its positive power, which is included in $\widehat{E}\widehat{E}$ and $1/\widehat{\mu}^3$, appears in front of \widehat{F} , the initial singularity appears. We can understand this fact as follows. For simplicity, we here assume that there is a constraint equation as $C = FV = 0$ classically. In quantum theory, there are two choices of the operator ordering for the constraint, and then the action of the constraint operators $\widehat{C}_1 = \widehat{V}\widehat{F}$ and $\widehat{C}_2 = \widehat{F}\widehat{V}$ on the state $|v\rangle$ is given by

$$\widehat{C}_1 |v\rangle = \widehat{V}\widehat{F} |v\rangle = -\frac{1}{16} (V_{v+4}|v+4\rangle - 2V_v|v\rangle + V_{v-4}|v-4\rangle), \quad (4.13)$$

$$\widehat{C}_2 |v\rangle = \widehat{F}\widehat{V} |v\rangle = -\frac{V_v}{16} (|v+4\rangle - 2|v\rangle + |v-4\rangle). \quad (4.14)$$

Then, the constraint equations for $\Phi(v)$ become

$$V_v(\Phi(v+4) - 2\Phi(v) + \Phi(v-4)) = 0, \quad (4.15)$$

for \widehat{C}_1 , and

$$V_{v+4}\Phi(v+4) - 2V_v\Phi(v) + V_{v-4}\Phi(v-4) = 0, \quad (4.16)$$

for \widehat{C}_2 , respectively. In Eq. (4.15), there is the same eigenvalue V_v of the volume operator in each term, and then all coefficients vanish for $v = 0$. For this reason, in this case, we cannot determine $\Phi(-4)$ from $\Phi(4)$ and $\Phi(0)$, and do not have the unique evolution. On the other hand, in Eq. (4.16), the left hand side does not disappear even for $v = 0$. Thus, we can determine the unique solution beyond $v = 0$, and therefore there is no singularity.

V. DISCUSSION

To make the present analysis complete we also need to discuss the matter Hamiltonian C_{matter} . For simplicity, we first focus on the equi-volume discretisation. Matter fields can be incorporated by introducing the dependence of the wave function on the matter fields such as $\Phi(v, \phi)$. Then, we can see that the presence of the matter fields does not greatly change the discussion. For example, suppose we choose Eq. (4.12a) as the gravitational part of the difference equation. Then, for $\Phi(v, \phi)$ we obtain the following evolution equation

$$\begin{aligned} &|v+4| ||v+3| - |v+5| \Phi(v+4, \phi) - \left(2|v| ||v-1| - |v+1| - \frac{128\pi}{81} \gamma^3 \frac{l_{\text{Pl}}^2}{K^2} \Lambda |v| \right) \Phi(v, \phi) \\ &+ |v-4| ||v-5| - |v-3| \Phi(v-4, \phi) = -48Kl_{\text{Pl}}\sqrt{\pi}\gamma^3\widehat{C}_{\text{matter}}\Phi(v, \phi), \end{aligned} \quad (5.1)$$

where we have used the constraint equation $C_{\text{grav}} + C_{\text{matter}} = 0$. As is explicitly shown in Appendix C, for general matter fields with an exceptional case, the right hand side of Eq. (5.1) is proportional to $\Phi(v, \phi)$ and the coefficient vanishes for $v = 0$. This means that the presence or absence of the singularity does not depend on the matter fields in general. It depends on the operator ordering of the gravitational Hamiltonian constraint. This is also true for the equi-area discretisation.

Whether the wave function recovers the smoothness in the large volume limit strongly depends on the choice of the discretisation as well as the form of the matter fields. Actually, this problem is already studied well in detail by Nelson and Sakellariadou [11, 12]. In this context, the present paper has shown that if we only include the cosmological constant, the large volume limit is problematic in the equi-area discretisation but this problem is resolved in the equi-volume discretisation. In reality, the cosmological constant model with each discretisation falls into some particular set of the parameter values in their notation and we can find that clearly our result is consistent with theirs. On the other hand, we have generated the solution of the finite difference equation for both discretisations and shown how problematic the equi-area discretisation is and how nicely the equi-volume discretisation sorts this out. Since this behaviour can be explained completely by taking the large volume limit of the discretised Hamiltonian constraint equations and the choice of the operator ordering does not affect this limit, it is clear that the large volume limit is insensitive to the choice of the operator ordering.

VI. CONCLUSION

We have investigated a homogeneous, isotropic and spatially flat universe with the cosmological constant in the context of LQC. In particular, we have studied theoretical ambiguities in the quantisation of the Hamiltonian, which arise in the operator ordering and the discretisation and are hard to fix within the framework of LQC. We focus on two important features of LQC, the absence of the initial singularity and the large volume limit. We have shown that the absence of the initial singularity strongly depends on the choice of the operator ordering. Therefore, the requirement for the absence of the singularity can potentially make the ordering ambiguity very small. Furthermore, we have found a general ordering rule required for the absence of the singularity. On the other hand, the choice of the discretisation is crucial when we consider the large volume limit. We have demonstrated two typical choices of the discretisation, the equi-area and equi-volume ones. Then, we have shown that in the former case there arises a serious problem in the physical interpretation of the wave function as a continuous function in the large volume limit and also that this problem is resolved in the latter case. It is clear that we cannot fix these ambiguities only from the present results. However, if we can deduce the physical implications of full LQG even qualitatively, we will be able to fix the ambiguities of LQC as the phenomenological realisation of full LQG in the minisuperspace model.

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Appendix A: Wheeler-De Witt equation and its general solution

Here, we summarise the WDW theory for the flat FRW universe with the cosmological constant. In terms of the connection-triad variables c and p , the Poisson bracket takes the form

$$\{c, p\} = \frac{8\pi G\gamma}{3}, \quad (\text{A1})$$

and the Hamiltonian constraint is written as

$$C_{\text{grav}} = \frac{1}{16\pi\gamma^2 G} \left(-6c^2\sqrt{|p|} + 2\gamma^2\Lambda|p|^{\frac{3}{2}} \right) = 0. \quad (\text{A2})$$

To quantise the system, Dirac's method is used in the WDW theory. That is, the Poisson bracket (A1) is replaced by the commutation relation between the operators corresponding to the canonical pair:

$$[\hat{c}, \hat{p}] = \frac{8i\pi l_{\text{Pl}}^2 \gamma}{3}, \quad (\text{A3})$$

and the classical constraint (A2) is promoted to a constraint for physical quantum states: $\hat{C}_{\text{grav}}\Psi = 0$. This quantum constraint is called the WDW equation. We here consider the following three types of the operator ordering for the Hamiltonian constraint:

$$\hat{C}_{\text{grav}}^{(1)} = \frac{1}{16\pi\gamma^2 l_{\text{Pl}}^2} \left(-6\hat{c}^2\sqrt{|\hat{p}|} + 2\gamma^2\Lambda|\hat{p}|^{\frac{3}{2}} \right), \quad (\text{A4a})$$

$$\hat{C}_{\text{grav}}^{(2)} = \frac{1}{16\pi\gamma^2 l_{\text{Pl}}^2} \left(-6\sqrt{|\hat{p}|}\hat{c}^2 + 2\gamma^2\Lambda|\hat{p}|^{\frac{3}{2}} \right), \quad (\text{A4b})$$

$$\hat{C}_{\text{grav}}^{(3)} = \frac{1}{16\pi\gamma^2 l_{\text{Pl}}^2} \left(-6\hat{c}\sqrt{|\hat{p}|}\hat{c} + 2\gamma^2\Lambda|\hat{p}|^{\frac{3}{2}} \right). \quad (\text{A4c})$$

If we take the ordinary Schrödinger representation, where \hat{p} and \hat{c} respectively act as multiplication and differentiation:

$$\hat{p}\Psi = p\Psi, \quad \hat{c}\Psi = \frac{8i\pi l_{\text{Pl}}^2 \gamma}{3} \frac{d\Psi}{dp}, \quad (\text{A5})$$

the quantum constraints (A4a)-(A4c) yield the corresponding WDW equations

$$\hat{C}_{\text{grav}}^{(1)}\Psi^{(1)} = \frac{8\pi l_{\text{Pl}}^2}{3} \left(\sqrt{|p|} \frac{d^2\Psi^{(1)}}{dp^2} + \frac{\text{sgn}(p)}{\sqrt{|p|}} \frac{d\Psi^{(1)}}{dp} - \frac{1}{4}|p|^{-\frac{3}{2}}\Psi^{(1)} \right) + \frac{\Lambda}{8\pi l_{\text{Pl}}^2} |p|^{\frac{3}{2}}\Psi^{(1)} = 0, \quad (\text{A6a})$$

$$\hat{C}_{\text{grav}}^{(2)}\Psi^{(2)} = \frac{8\pi l_{\text{Pl}}^2}{3} \sqrt{|p|} \frac{d^2\Psi^{(2)}}{dp^2} + \frac{\Lambda}{8\pi l_{\text{Pl}}^2} |p|^{\frac{3}{2}}\Psi^{(2)} = 0, \quad (\text{A6b})$$

$$\hat{C}_{\text{grav}}^{(3)}\Psi^{(3)} = \frac{8\pi l_{\text{Pl}}^2}{3} \left(\sqrt{|p|} \frac{d^2\Psi^{(3)}}{dp^2} + \frac{\text{sgn}(p)}{2\sqrt{|p|}} \frac{d\Psi^{(3)}}{dp} \right) + \frac{\Lambda}{8\pi l_{\text{Pl}}^2} |p|^{\frac{3}{2}}\Psi^{(3)} = 0. \quad (\text{A6c})$$

The general solutions of the WDW equations (A6a)-(A6c) for $p \geq 0$ are given by

$$\Psi^{(1)} = p^{-\frac{1}{2}} \left[C_1 \text{Ai} \left(-\alpha_3^{\frac{1}{3}} p \right) + C_2 \text{Bi} \left(-\alpha_3^{\frac{1}{3}} p \right) \right], \quad (\text{A7a})$$

$$\Psi^{(2)} = C_1 \text{Ai} \left(-\alpha_3^{\frac{1}{3}} p \right) + C_2 \text{Bi} \left(-\alpha_3^{\frac{1}{3}} p \right), \quad (\text{A7b})$$

$$\Psi^{(3)} = p^{\frac{1}{4}} \left[C_1 \text{J}_{-\frac{1}{6}} \left(\frac{2}{3} \sqrt{\alpha_3} p^{\frac{3}{2}} \right) + C_2 \text{J}_{\frac{1}{6}} \left(\frac{2}{3} \sqrt{\alpha_3} p^{\frac{3}{2}} \right) \right], \quad (\text{A7c})$$

where C_1 and C_2 are arbitrary constants, Ai and Bi are the Airy functions, $J_{\pm\frac{1}{6}}$ is the Bessel function, and we have defined $\alpha_3 := 3\Lambda/(8\pi l_{\text{Pl}}^2)^2$.

Appendix B: Large volume limit of the difference equations

Here, we consider the large volume limit of $\langle\mu|\hat{C}_{\text{grav}}|\Psi\rangle$, and then we shall show that it corresponds to the WDW equation. First, we consider the operator orderings (3.3) and (3.5) in the equi-area discretisation. The operator ordering (3.3) yields

$$\begin{aligned} \langle\mu|\hat{C}_{\text{grav}}|\Psi\rangle &= \frac{1}{16\pi^2 l_{\text{Pl}}^2 \gamma^2} \frac{3}{8\pi\gamma l_{\text{Pl}}^2 \mu_0^3} \left[|V_{\mu+5\mu_0} - V_{\mu+3\mu_0}| \Psi(\mu + 4\mu_0) \right. \\ &\quad \left. - \left(2|V_{\mu+\mu_0} - V_{\mu-\mu_0}| - \frac{16\pi\gamma^3 l_{\text{Pl}}^2 \mu_0^3}{3} \Lambda V_\mu \right) \Psi(\mu) + |V_{\mu-3\mu_0} - V_{\mu-5\mu_0}| \Psi(\mu - 4\mu_0) \right]. \end{aligned} \quad (\text{B1})$$

For $\mu \gg \mu_0$, we can expand $(V_{\mu+L\mu_0} - V_{\mu+M\mu_0})$ around μ_0 as follows:

$$\begin{aligned} V_{\mu+L\mu_0} - V_{\mu+M\mu_0} &= \left(\frac{8\pi\gamma l_{\text{Pl}}^2}{6} \right)^{3/2} \mu^{3/2} \left\{ \frac{3}{2}(L - M) \frac{\mu_0}{\mu} + \frac{3}{8}(L^2 - M^2) \left(\frac{\mu_0}{\mu} \right)^2 \right. \\ &\quad \left. - \frac{1}{16}(L^3 - M^3) \left(\frac{\mu_0}{\mu} \right)^3 + O\left(\left(\frac{\mu_0}{\mu} \right)^4 \right) \right\}. \end{aligned} \quad (\text{B2})$$

Substituting Eq. (B2) into Eq. (B1), we obtain

$$\begin{aligned} \langle\mu|\hat{C}_{\text{grav}}|\Psi\rangle &= \frac{1}{16\pi^2 l_{\text{Pl}}^2 \gamma^2} \frac{3}{8\pi\gamma l_{\text{Pl}}^2 \mu_0^3} \left(\frac{8\pi\gamma l_{\text{Pl}}^2}{6} \right)^{3/2} \mu^{3/2} \left[3 \left(\frac{\mu_0}{\mu} \right) \{ \Psi(\mu + 4\mu_0) - 2\Psi(\mu) + \Psi(\mu - 4\mu_0) \} \right. \\ &\quad + 6 \left(\frac{\mu_0}{\mu} \right)^2 \{ \Psi(\mu + 4\mu_0) - \Psi(\mu - 4\mu_0) \} - \frac{1}{8} \left(\frac{\mu_0}{\mu} \right)^3 \{ \Psi(\mu + 4\mu_0) - 2\Psi(\mu) + \Psi(\mu - 4\mu_0) \} \\ &\quad \left. - 6 \left(\frac{\mu_0}{\mu} \right)^3 \{ \Psi(\mu + 4\mu_0) + \Psi(\mu - 4\mu_0) \} + \frac{16\pi\gamma^3 l_{\text{Pl}}^2 \mu_0^3}{3} \Lambda \Psi(\mu) + O\left(\left(\frac{\mu_0}{\mu} \right)^4 \right) \right]. \end{aligned} \quad (\text{B3})$$

Assuming that the wave function varies sufficiently slowly and expanding the wave function $\Psi(\mu \pm 4\mu_0)$ around μ , we obtain

$$\Psi(\mu \pm 4\mu_0) = \Psi(\mu) \pm \frac{d\Psi(\mu)}{d\mu}(4\mu_0) + \frac{1}{2} \frac{d^2\Psi(\mu)}{d\mu^2}(16\mu_0^2) \pm \frac{1}{6} \frac{d^3\Psi(\mu)}{d\mu^3}(64\mu_0^3) + O\left(\mu_0^4 \frac{d^4\Psi(\mu)}{d\mu^4} \right). \quad (\text{B4})$$

Substituting Eq. (B4) into Eq. (B3), we obtain

$$\langle\mu|\hat{C}_{\text{grav}}|\Psi\rangle = \frac{\sqrt{3}}{\sqrt{\pi^3 \gamma^3 l_{\text{Pl}}}} \left[\frac{d^2}{d\mu^2}(\sqrt{\mu}\Psi(\mu)) + \frac{\pi\gamma^3 l_{\text{Pl}}^2}{9} \mu^{3/2} \Lambda \Psi(\mu) + O(\mu_0) \right]. \quad (\text{B5a})$$

Because $\mu \propto p$, this equation is just the WDW equation as in Appendix A. Similarly, we consider the large volume limit of $\langle\mu|\hat{C}_{\text{grav}}|\Psi\rangle$ in the operator ordering (3.5), and then we obtain the WDW equation

$$\langle\mu|\hat{C}_{\text{grav}}|\Psi\rangle = \frac{\sqrt{3}}{\sqrt{\pi^3 \gamma^3 l_{\text{Pl}}}} \left[\sqrt{\mu} \frac{d^2}{d\mu^2} \Psi(\mu) + \frac{\pi\gamma^3 l_{\text{Pl}}^2}{9} \mu^{3/2} \Lambda \Psi(\mu) + O(\mu_0) \right]. \quad (\text{B5b})$$

Second, we calculate the large volume limit of $\langle v|\hat{C}_{\text{grav}}|\Psi\rangle$ in the operator orderings (4.12a) - (4.12d) in the equi-volume discretisation. To do this, we here assume that $|v| \gg 1$ and $\Phi(v)$ varies sufficiently slowly. Then, we obtain

the WDW equations from the operator orderings (4.12a) - (4.12d), respectively, as follows:

$$\frac{27}{8l_{\text{Pl}}\gamma^{3/2}}\sqrt{\frac{8}{6\pi}}K\left[\frac{d^2}{dv^2}(|v|\Phi(v)) + \frac{4\pi}{81}\gamma^3\frac{l_{\text{Pl}}^2}{K^2}\Lambda|v|\Phi(v) + O\left(\frac{d^3\Phi(v)}{dv^3}\right)\right], \quad (\text{B6a})$$

$$\frac{27}{8l_{\text{Pl}}\gamma^{3/2}}\sqrt{\frac{8}{6\pi}}K\left[|v|\frac{d^2}{dv^2}\Phi(v) + \frac{4\pi}{81}\gamma^3\frac{l_{\text{Pl}}^2}{K^2}\Lambda|v|\Phi(v) + O\left(\frac{d^3\Phi(v)}{dv^3}\right)\right], \quad (\text{B6b})$$

$$\frac{27}{8l_{\text{Pl}}\gamma^{3/2}}\sqrt{\frac{8}{6\pi}}K\left[|v|\frac{d^2}{dv^2}\Phi(v) + \frac{4\pi}{81}\gamma^3\frac{l_{\text{Pl}}^2}{K^2}\Lambda|v|\Phi(v) + O\left(\frac{d^3\Phi(v)}{dv^3}\right)\right], \quad (\text{B6c})$$

$$\frac{27}{8l_{\text{Pl}}\gamma^{3/2}}\sqrt{\frac{8}{6\pi}}K\left[\frac{d^2}{dv^2}(|v|\Phi(v)) + \frac{4\pi}{81}\gamma^3\frac{l_{\text{Pl}}^2}{K^2}\Lambda|v|\Phi(v) + O\left(\frac{d^3\Phi(v)}{dv^3}\right)\right]. \quad (\text{B6d})$$

Appendix C: Matter Hamiltonian constraint

Here, we shall discuss the matter Hamiltonian operator. We assume that the matter Hamiltonian constraint can be written by $a^r\epsilon(a, \phi)$ for arbitrary matter fields ϕ , where r is a constant and $\epsilon(a, \phi)$ is a function of the matter fields and the scale factor such that $\epsilon(a, \phi)$ has a nonzero and finite limit for $a \rightarrow 0$.

First, we consider the case for $r < 0$. Classically, the matter Hamiltonian diverges for $a \rightarrow 0$ due to the inverse scale factor. In LQG, such a divergence can be regularised by Thiemann's prescription [18]: we multiply the matter Hamiltonian constraint by $1^m = \left(\det e_a^i / \sqrt{|\det E|}\right)^m$, where m can be chosen such that we obtain the positive power of the volume factor. Similarly, we regularise the inverse scale factor in LQC as follows [14]. The classical Poisson bracket takes the form

$$\left\{c, V^{\frac{2l}{3}}\right\} = \text{sgn}(p)\frac{8\pi\gamma Gl}{3}|p|^{l-1}, \quad (\text{C1})$$

where we have used $V = |p|^{3/2}$, and l is the ambiguity parameter similar to m in LQG. Notice that if we choose $0 < l < 1$, the right hand side denotes the inverse power of p , while the left hand side involves the positive power of the volume. Using this property, we rewrite the inverse scale factor a^{-1} as

$$a^{-1} = \frac{V_0^{\frac{1}{3}}}{\sqrt{|p|}} = \left(\frac{3\text{sgn}(p)}{8\pi\gamma Gl}\left\{c, V^{\frac{2l}{3}}\right\}\right)^{\frac{1}{2(1-l)}}V_0^{\frac{1}{3}}, \quad (\text{C2})$$

where we used $|p| = V_0^{2/3}a^2$. Then, the matter Hamiltonian becomes

$$\begin{aligned} C_{\text{matter}} &= a^r\epsilon(a, \phi) = \left[\frac{1}{\sqrt{|p|}}\right]^{-r}V_0^{-\frac{r}{3}}\epsilon(a, \phi) \\ &= \left[\frac{3\text{sgn}(p)}{8\pi\gamma Gl}\left\{c, V^{\frac{2l}{3}}\right\}\right]^{-\frac{r}{2(1-l)}}V_0^{-\frac{r}{3}}\epsilon(a, \phi). \end{aligned} \quad (\text{C3})$$

This classical formula can be represented exactly in terms of holonomies as follows:

$$C_{\text{matter}} = \left[\frac{\text{sgn}(p)}{4\pi\gamma Gl\bar{\mu}}\text{Tr}\left(\sum_i \tau^i h_i^{(\bar{\mu})}\left\{h_i^{(\bar{\mu})-1}, V^{\frac{2l}{3}}\right\}\right)\right]^{-\frac{r}{2(1-l)}}V_0^{-\frac{r}{3}}\epsilon(a, \phi), \quad (\text{C4})$$

and we can quantise this Hamiltonian immediately by replacing the Poisson bracket $\{\bullet, \bullet\}$ with $-i[\bullet, \bullet]$. Using $G = l_{\text{Pl}}^2$ and Eq. (4.4), after some calculation, we obtain

$$\hat{C}_{\text{matter}} = \left[-\frac{3i(\text{sgn}(p))}{4\pi\gamma l_{\text{Pl}}^2 l}\left(\frac{6}{8\pi l_{\text{Pl}}^2 \gamma}\right)^{1/2}\left(\frac{K\hat{V}}{\sqrt{3}}\right)^{\frac{1}{3}}\left(\sin\left(\frac{\bar{\mu}c}{2}\right)V^{\frac{2l}{3}}\cos\left(\frac{\bar{\mu}c}{2}\right) - \cos\left(\frac{\bar{\mu}c}{2}\right)V^{\frac{2l}{3}}\sin\left(\frac{\bar{\mu}c}{2}\right)\right)\right]^{-\frac{r}{2(1-l)}}V_0^{-\frac{r}{3}}\widehat{\epsilon(a, \phi)}. \quad (\text{C5})$$

Then, the matter Hamiltonian operator acts on $|v\rangle$ as

$$\hat{C}_{\text{matter}}|v\rangle = \left[\frac{3\text{sgn}(p)}{8\pi\gamma l_{\text{Pl}}^2 l} \left(\frac{6}{8\pi l_{\text{Pl}}^2 \gamma} \right)^{1/2} \left(\frac{KV_v}{\sqrt{3}} \right)^{\frac{1}{3}} \left(V_{v+1}^{\frac{2l}{3}} - V_{v-1}^{\frac{2l}{3}} \right) \right]^{-\frac{r}{2(1-l)}} V_0^{-\frac{r}{3}} \epsilon_0(a, \phi) |v\rangle, \quad (\text{C6})$$

where $V_v = (8\pi\gamma l_{\text{Pl}}^2/6)^{3/2} |v|/K$ and $\epsilon_0(a, \phi)$ is an eigenvalue of $\widehat{\epsilon(a, \phi)}$. Therefore, $|v\rangle$ is an eigenstate of \hat{C}_{matter} , and its eigenvalue vanishes for $v = 0$. Therefore, substituting this into Eq. (5.1), since the eigenvalue of the matter Hamiltonian operator vanishes for $v = 0$, we can uniquely determine the coefficients $\Phi(v, \phi)$ except for $\Phi(0, \phi)$. In conclusion, the matter Hamiltonian operator does not affect the absence or presence of the singularity for $r < 0$.

Second, we consider the case with $r = 0$. In this case, the matter Hamiltonian is given by $C_{\text{matter}} = \epsilon(a, \phi)$. Thus, the matter Hamiltonian operator acts on the state $|v\rangle$ as

$$\hat{C}_{\text{matter}}|v\rangle = \epsilon_0(a, \phi) |v\rangle. \quad (\text{C7})$$

Then, $|v\rangle$ is an eigenstate of \hat{C}_{matter} but in this case its eigenvalue does not vanish even for $v = 0$. Substituting this into Eq. (5.1), we find that we cannot uniquely determine $\Phi(0, \phi)$ from this equation and hence cannot obtain the unique wave function $\Phi(v, \phi)$ beyond $v < 0$. Therefore, in this case, even though there is no initial singularity without matter fields, there appears the initial singularity due to the presence of the matter fields.

Finally, for $r > 0$, the matter Hamiltonian becomes $C_{\text{matter}} = V^{r/3} \epsilon(a, \phi)$. Thus, the matter Hamiltonian operator acts on the state $|v\rangle$ as

$$\hat{C}_{\text{matter}}|v\rangle = V_v^{\frac{r}{3}} \epsilon_0(a, \phi) |v\rangle. \quad (\text{C8})$$

Therefore, $|v\rangle$ is an eigenstate of \hat{C}_{matter} , and its eigenvalue vanishes for $v = 0$. Similarly to the case of $r < 0$, the matter Hamiltonian does not affect the absence or presence of the singularity.

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